Advanced Python in HEP Starterkit 2021

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... building on the existing starterkit material

Installing Python

- Recommended: use anaconda/miniconda, always with environments
 - Package installer that can handle way more:
 - Install ROOT (within few minutes, no kidding!)
 - Have multiple Python and package versions

Attention:

- can grow big (~GB)! Install to "data" folder with still fast I/O rate, not home
- Disable base environment (see installer)
- Add conda-forge to channels

Let's dive in!

Python

- Interpreted language
 - Every line gets compiled, then executed
 → no need for pre-compilation
 - Very dynamic, a lot of user-friendly features
- #1 language in Data Analysis, most popular language in general
- General purpose programming language
- Heavily used (guesstimated > 50%) inside LHCb, CMS, others...

Python is easy

Python is slow

- Python is easy
 - Simple to learn, just use it

- Python is slow
 - Unfortunately, therefore C++ must be used for large data

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"Driving a car is easy. Just push the power. Any 5 year old can do..."

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"Driving a car is easy. Just push the power. Any 5 year old can do..."

(Which is "true" compared to e.g. a bicycle)

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"Driving a car is easy. Just push the power. Any 5 year old can do..."

Problem: accidents <=> bugs

(see e.g. this talk)

Python is beautiful!

- Clean, powerful and well designed
- ... and yes, less to care about

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A Ferrari is slow...

Python is slow

A Ferrari is slow...

True, if you transport goods, compared to a truck

Python is slow

"Writing C++ code, that does heavy number crunching, with Python syntax and executing it with a Python interpreter is slow"

True!

-Python is slow

Python is a high level language

Python

C++

Compiler and more

Python is slow

Python is a fast, high level language

- It uses C++/Fortran code for computations
- No need for manual implementation e.g. just add vectors

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Python in HEP

User base:

- Many C++ users, Python still "newish" (and Python-writing-in-C++)
 → not every script is perfect Python
- Very useful for data analysis
 - Shared ecosystem with open-source community
 - HEP ecosystem new, strong in last few years
- Many packages in Python for HEP
 - → see Scikit-HEP
- ROOT can be used with Python

This lecture

• Ideal: fully planned lectures, well designed, perfect pace...

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- Everyone has a different Python level (and it's spread usually)
- average level of Python increases every year
- Python ecosystem changes rapidly

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Focus is on HEP in Python, there are some tutorials, but... let's find out together!

This lecture is...

...dynamic. Depending on you.

- More material available than time
- Follows somewhat online course

...not just an overview

- You will spend a lot of time with Python
- Some deeper understanding of critical parts

…interactive.

- Solve small problems and ask about the libraries
- Ask questions about concepts and code

This lecture is...

- (Introduction to classes?)
- Medium Python concepts
 - *, **; context manager, exceptions,...
 - (numpy, math libraries?)
- Basics of data handling and plotting
 - Uproot, pandas, cuts, plots...
- Multivariate analysis (machine learning)
 - BDT, uniformity, training and test
- Histograms and reweighting
- Likelihood fits and inference
 - Building models, fitting, significance
- Scikit-HEP diverse tools

Editors

- Vim or Emacs
- Simple editors like nano, gedit
- IDE (Integrated Development Environment)
 - Offers great support for so many things
 - Special mention: PyCharm

Learning a language

Languages

- Programming similar to natural language
- How to learn:
 - Grammar/Syntax + Rules
 - Practice
 - Time
- Be curious!
 - Ask yourself: what exactly is happening?
 - Try out: what if I do this?

Conventions

Can I write...

- Hel lo, i havearri ved
- Хелло, и хаве арривед.
- Hallo, ich bin angekommen.
 - ... if I wanna say "Hello, I have arrived."?

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No!

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Conventions:

- When there are several ways, we agree on one
- Make life easier for everyone!

There should be one – and preferably only one – obvious way to do it.

Python conventions

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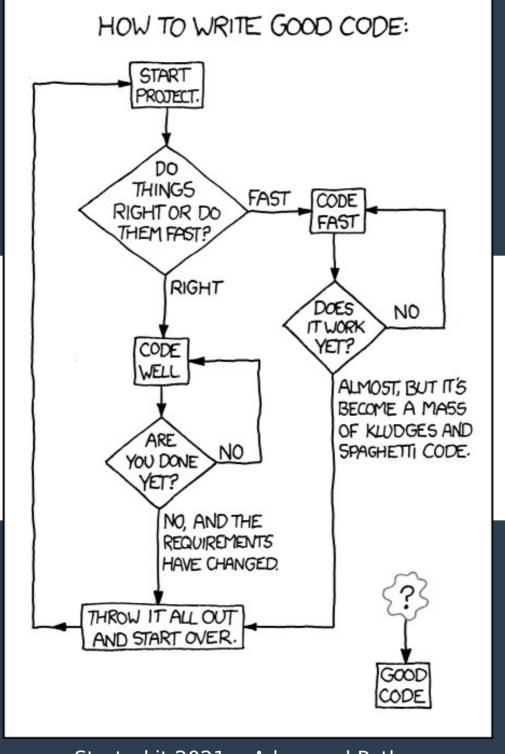
Python lives from conventions

- Because it is so powerful and let's you do a lot
 "We are consenting adults"
- PEP8: style-guide (many auto checkers)
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 - >>> import this

writing code is more than writing code



...(although I speak English!)

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 - ... and a language to "implement it"

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- Book author
 ⇔ software engineer
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 - Knowing how to program ≠ knowing the language
- OOP, composition, interfaces, protocols, CI/CD, unittests, responsibilities, stateful, VCS, code review, legacy, open-close, forward/backwards compatibility, DRY, etc.

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 OOP, coupling, interfaces, protocols, CI/CD, unittests, responsibilities, stateful, VCS, code review, legacy, forward/backwards compatibility, DRY, etc.

We do not need to know all that, but:

- Be aware of your limits
- We do not need (and should not!)
 reinvent programming
 - ... it's invented, let's learn from the right people.

Vectorization

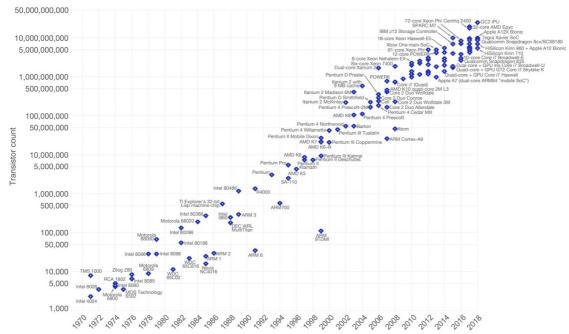
Moore's law

- every 1.5 year, the CPU power doubles
- Stated in the 70s → just holds

Moore's Law – The number of transistors on integrated circuit chips (1971-2018)



Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important as other aspects of technological progress – such as processing speed or the price of electronic products – are linked to Moore's law.



Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count)
The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

Licensed under CC-BY-SA by the author Max Roser

Well, actually...

- It states that the clock frequency doubles
- One problem: heat dissipation ~ f^3
 - Not a problem until 2000's
 - Now a problem: frequency stuck at GHz
- But: parallelization helps (Moore's law still basically true)

Paralellization

- You need many exercises to split amongst students
- 100 students but giving them 1 exercise (serial) after the other is useless
- Idea: think vectorized
 - Vector operations automatically include multiple operations at once
 - Hardware like GPU built for massively parallel execution of the same operation on points

Sometimes we can cheat

- Some libraries can (sometimes) convert forloops to vectors
- Learn to think vectorized!
 - (not so easy if used to for-loops)
- Code vectorized
 - Pandas, numpy, TensorFlow etcetcetc.
- Key to speed

Number crunching!